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14. ABSTRACT Simulations of a model configuration of a lean direct injection (LDI) gas turbine combustor were performed to assess the effects of fuel spray modeling in predicting combustion instability. Concurrently, experimental data were obtained at the same conditions in a test combustor with the same configuration for comparison. To improve the simulation predictions, fuel spray modeling was tuned and assessed in two major steps. First, focus is put on the Weber number-adaptive hybrid model that describes the secondary atomization. Tuning the model constants over a finite range does not have a significant effect on the predictions. Second, specified fuel spray distributions are tested to replace the linear stability primary breakup model (LISA). Both uniform and log-normal distributions are used with different mean drop diameters. A better match between pressure amplitude could be achieved by specifying a spray drop distribution, but the predicted dominant modes (3L/4L and 1T) seemed to be very sensitive to the distributions applied.					
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Effects of Fuel Spray Modeling on Combustion Instability Predictions in a Single-Element Lean Direct Injection (LDI) Gas Turbine Combustor

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Simulations of a model configuration of a lean direct injection (LDI) gas turbine combustor were performed to assess the effects of fuel spray modeling in predicting combustion instability. Concurrently, experimental data were obtained at the same conditions in a test combustor with the same configuration for comparison. To improve the simulation predictions, fuel spray modeling was tuned and assessed in two major steps. First, focus is put on the Weber number-adaptive hybrid model that describes the secondary atomization. Tuning the model constants over a finite range does not have a significant effect on the predictions. Second, specified fuel spray distributions are tested to replace the linear stability primary breakup model (LISA). Both uniform and log-normal distributions are used with different mean drop diameters. A better match between pressure amplitude could be achieved by specifying a spray drop distribution, but the predicted dominant modes (3L/4L and 1T) seemed to be very sensitive to the distributions applied.

I. Introduction and Background

Lean direct injection is a promising combustor concept where liquid fuel is injected and mixed with air rapidly in a short distance. In the configuration used here, a subsonic venturi is used in combination with an air swirler and pressure atomizer to provide highly inertial forces for atomization and mixing. It was developed as an alternative to Lean Prevaporized Premixed (LPP) combustion for improved low NO_x emissions that eliminates issues encountered in LPP combustion such as auto-ignition and flash-back. Yi and Santavicca's experimental study indicated similarity of flame spectra in an LDI combustor to those in observed in lean premixed gaseous combustion¹. However, as with other lean-burning combustors, the LDI combustor can be susceptible to self-excited combustion instabilities as the equivalence ratio approaches fuel lean conditions. Under such conditions, the combustion response can be coupled with the acoustic fluctuations to sustain combustion instabilities in the combustor. In the experimental study of Cohen et al.², oscillating levels of pressure at longitudinal acoustic frequencies were reported within 3% of the mean chamber pressure. In Yi and Santavicca's experiment, self-excited longitudinal mode combustion dynamics has been reported at pressure amplitudes of 5-7% of the mean chamber pressure¹. More recent parametric experimental studies in Purdue reported pressure oscillations at total peak-to-peak amplitude from 3% to 20% of the mean chamber pressure by varying geometry lengths, inlet air temperatures and equivalence ratios³.

Computational simulations of the LDI concept requires the capability to describe multi-phase flow physics, the influence of which in atomization, vaporization and generated heat release makes it a critical factor for predictions

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of combustion instability. In our particular LDI configuration, a pressure-swirl atomizer has been used and extensive experimental and computational work has been done to characterize the internal and external flow through the atomizer. The liquid sheet emanating from a simplex pressure-swirl atomizer has been studied by Jeng et al.⁴ both experimentally and computationally. Cousin et al.⁵ measured drop sizes in a pressure swirl atomizer and compared to predicted results based on the coupling of linear theory with the maximum-entropy formalism. Many examples of computational studies of an LDI combustor with fuel spray modeling can also be found in the literature. Patel and Menon⁶ performed large eddy simulation (LES) on a LDI element using a single drop injection model with atomization described by Reitz's Kelvin-Helmholtz (KH) breakup model^{7,8} and found that the atomization process has a major impact on the fuel evaporation in the vicinity of the injector. Recently, Kim and Menon⁹ applied the same approach to study the characteristics of longitudinal combustion instability in an LDI combustor, using the same experimental configuration as in the present article. Dewanji et al.¹⁰ conducted the Reynolds-averaged Navier Stokes (RANS) simulation for their multipoint LDI combustor also using the KH breakup model.

Our present work covers concurrent experimental and computational studies of an unstable LDI configuration that has been studied at Purdue University since 2011. The overall research program is aimed in part at validating high-fidelity simulations using the benchmark experiments and in part at elucidating the underlying physical phenomena that govern the occurrence of combustion instabilities. The experiments involve a single injector element in a longitudinal mode combustor with well characterized inflow conditions and a choked nozzle exit condition. Varying parameters such as the length of the air plenum, the combustor length, swirl velocity, the fuel-air mixture ratio and the fuel-nozzle location relative to the chamber, different modes and amplitudes of combustion stability have been observed. Detailed diagnostics such as Phase Doppler Anemometry, Particle Image Velocimetry (PIV), OH-PLIF and high-speed pressure measurements are being performed to get quantitative data in the chamber. The validation study and the associated physical understanding are important precursors for the model to be used with confidence in the design of stable LDI configurations.

The basic model used in the study involves time-dependent calculations of the Navier-Stokes equations using a detached eddy simulations (DES) model of the turbulence, finite-rate chemical kinetics and various models for primary and secondary atomization of the fuel. Preliminary studies and comparisons between experiment and simulation have been done by Yoon et al.¹¹ Specifically, inlet geometry effects were investigated to minimize the effect of the inlet on downstream hydrodynamic unsteadiness. Parametric assessments were performed using two-dimensional axisymmetric simulations. The simulations were performed using specified log-normal distributed drop injection both with and without Reitz's breakup model^{7,8} to describe the secondary atomization. Different equivalence ratios were used to compare with experiment data. Additionally, details of the fuel spray modeling effects on the combustion dynamics predictions have also been studied in Ref 12. The spray characteristics (spray angle, drop size distribution etc.) were compared between the experimental measurements and simulation results at atmospheric pressure conditions in an unconfined geometry. Three fuel spray injection models, viz., Log Normal Distributed Drop Injection Model, Single Drop Injection Model and Hollow Cone Injection Model, have been evaluated for their capabilities of predicting combustion instability and matching experiment results.

In a follow-up study, an enhanced hybrid fuel spray model was developed to provide a more sophisticated description of the spray atomization¹³. A hybrid model was developed that combines the Linear Instability Sheet Atomization (LISA) model for primary atomization with the Taylor Analogy Breakup (TAB), Kelvin-Helmholtz, and Rayleigh-Taylor models for secondary atomization. The effects of the above fuel spray modeling are summarized in Table 1 based on LDI simulations with fuel nozzle located at venturi throat. It was reported in Ref. 14 that simulations with the hybrid model matched the experimental pressure measurements (dominant frequencies and amplitudes) reasonably well when the fuel nozzle was located upstream of the venturi throat, but the pressure amplitude was severely under-predicted when the fuel nozzle was located at the throat. As shown in Fig.1, the experimental measurements show higher pressure amplitude when the fuel nozzle is at the venturi throat than when it is located upstream of the venturi throat, but the computational results show the opposite trend. Detailed investigations of underlying physical phenomena leading to combustion instabilities were further conducted by Huang et al.¹⁵ for the low equivalence ratio case ($\Phi = 0.36$) which showed very good agreement with experimental data.

The present paper is focused on continuing the work reported in Refs. 12 and 14. The specific objective is to carefully assess the effects of fuel spray modeling on the combustion instability predictions and to improve the models so that they can better predict the stability results for the case with fuel nozzle at the venturi throat. Simulation results are compared between cases with different fuel nozzle locations to obtain some basic understanding of potential modeling issues that exist in the current simulations. Then model evaluations and

intended prediction improvement are performed in two major steps. First, model constants used in the secondary breakup model are tuned to reduce the spray drop size and accelerate the breakup process. The predicted pressure signals are compared against experiment measurement to evaluate the effects of secondary breakup models. Gaseous fuel and heat release distributions are compared further to study the modeling influences on combustion response. Second, focus is moved to the primary breakup stage. A specified drop distribution is used to replace the LISA model for primary atomization. Different distributions are applied to study their effects on the predicted pressure signals and the combustion response. The following sections of the paper present the pertinent details of the computational model, followed by the results of the two parametric studies mentioned above and concludes with a summary of the major findings and suggested directions for future work.

Operating Conditions	Case Name	Total peak-to-peak pressure amplitude (%)	Dominant Acoustic Mode	Secondary Atomization Model
$T_{\text{air}} = 800\text{K}$, $\Phi = 0.6$	Experiment	15	4L	/
$T_{\text{air}} = 750\text{K}$, $\Phi = 0.6$	Case 1: Log Normal Distributed Drop Injection	11	1L	No
	Case 2: Single Drop Injection	7	2L	KH
	Case 3: Hollow Cone Injection	0.24	4L	KH
$T_{\text{air}} = 800\text{K}$, $\Phi = 0.6$	Case 4: LISA + Hybrid Secondary Breakup Model	0.5	3L	Hybrid TAB/KH/RT

Table 1. Summary of fuel spray modeling effects on predicting combustion instability (fuel nozzle is located at the venturi throat) ¹⁴.

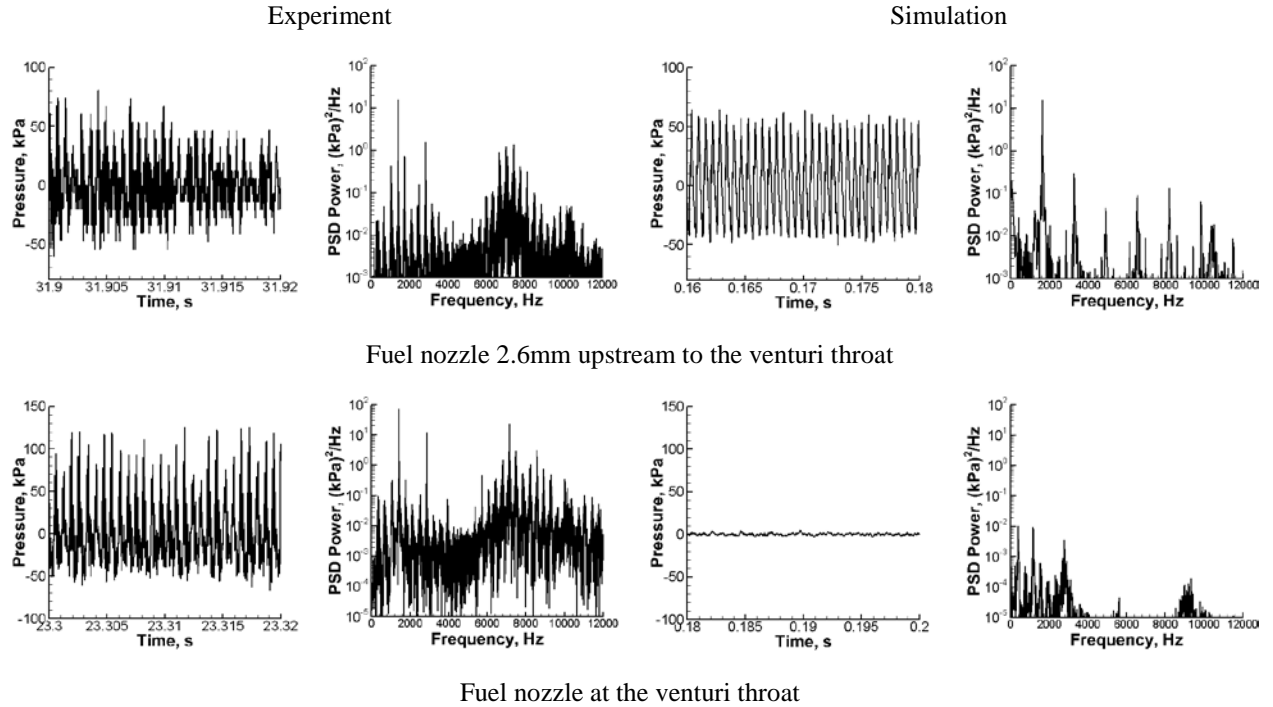


Figure 1. Experiment and simulation comparison for $T_{\text{air}} = 800\text{K}$ and $\Phi = 0.6$ (simulations are performed using Case 4 model in Table 1) ¹⁴.

II. Overview of the Computational Model

A. Computational Framework

The computational platform for the present simulations is an in-house code, GEMS (General Equation and Mesh Solver)¹⁶⁻¹⁹. GEMS is a fully unstructured, density-based finite volume solver with a second-order numerical scheme and an implicit, dual time procedure for time-accuracy. The capabilities of the code for capturing combustion dynamics and estimating instabilities have been successfully demonstrated for rocket engine combustors.^{20, 21} GEMS solves the Navier-Stokes equations along with the energy and species equation. A dual-time formulation is used to eliminate approximate-factorization and linearization errors. Turbulence is modeled using a hybrid RANS/LES formulation^{22,23} where the near wall region is modeled using a two-equation $k-\omega$ model^{24,25}. Combustion is accounted for using a simplified two-step, five-species global reduced mechanism²⁶ with laminar finite rate kinetics as shown below,



B. Fuel Spray Model

Modeling of direct injection sprays for gas turbine engines has been developed for combustion dynamics problems. This method combines sub-models for atomizing, vaporizing and reacting sprays. Key physical events considered in the present model include free-surface jet in the atomizer, primary and secondary breakup, drop vaporization, mixing and burning. The models are implemented within an Lagrangian-Eulerian framework, where the droplet phase is described by Lagrangian dynamics and the vaporized fuel is input as a source term along with associated momentum and energy terms in the Eulerian gas-phase equations.

Details of the present fuel spray modeling implementation can be found in Yoon et al.¹¹⁻¹³ and here only a brief overview is given. There are three major models for the description of spray atomization: atomizer free surface flow, primary and secondary atomization models. The first model is to describe the atomizer free surface flow. Independent calculation of the free surface internal flow in the atomizer is used to provide the spray injection conditions of the Lagrangian spray particles. Ashraf and Jog's numerical model²⁷ is employed for the present study. This model directly solves the two phase flow using the Eulerian Volume-Of-Fluid (VOF) Method and provides the spray angle, liquid sheet thickness and velocity. This information is delivered to the primary atomization model, which is the second model. The primary atomization is described by the linear stability analysis of the liquid sheet proposed by Senecal et al.²⁸. Using the liquid sheet thickness and velocity, the most unstable wave length and maximum growth rate are determined by dispersion relation derived from linear stability theory, and ligament and drop sizes disintegrated from the liquid sheet are then calculated. Lagrangian drops produced by the primary atomization are defined at the exit plane of the atomizer and then undergo the secondary atomization process, which is in turn represented by the third model. For the secondary atomization process, the drops may be broken up by several kinds of modes. The secondary atomization model developed in the present study covers the full Weber number range typically encountered in gas turbine combustors. Depending on the Weber number range, appropriate secondary atomization models are applied that include the Taylor Analogy Breakup (TAB), Kelvin Helmholtz (KH) and Rayleigh-Taylor (RT) models.

For $11 < \text{We} < 40$, TAB model is applied, which was proposed by O'Rourke and Amsden²⁸ and is based on the classical analogy between an oscillating and distorting droplet and a spring mass system. It is regarded that the external, restoring and damping forces in a spring mass system correspond to the drag, surface tension and viscous forces in a drop oscillation and distortion process.

$$\frac{d^2 y}{dt^2} = \frac{C_f}{C_b} \frac{\rho_g}{\rho_l} \frac{u^2}{r^2} - \frac{C_k \sigma}{\rho_l r^3} y - \frac{C_d \mu_l}{\rho_l r^2} \frac{dy}{dt} \text{ where } y = \frac{x}{C_b r}$$

breakup occurs when $y > 1$

$$y(t) = We_c + e^{-(t/t_d)} \left[(y_0 - We_c) \cos(\omega t) + \frac{1}{\omega} \left(\frac{dy_0}{dt} + \frac{y_0 - We_c}{t_d} \right) \sin(\omega t) \right] \quad (2)$$

where $We_c = \frac{C_f}{C_k C_b} We$ and $\omega = \sqrt{\frac{C_k \sigma}{\rho_l r^3} - \left(\frac{C_d}{2 \mu_l \rho_l r^2} \right)^2}$

where $We_c = \frac{C_f}{C_k C_b} We$ and $\omega = \sqrt{\frac{C_k \sigma}{\rho_l r^3} - \left(\frac{1}{3} \right)^2}$

The recommended model constants from the literature are $C_b = 0.5$, $C_k = 8.0$, $C_d = 5.0$ and $C_f = 1/3$.

For $40 < We < 350$, the KH model is used. It was originally formulated by Reitz and is based on the Kelvin-Helmholtz (KH) instability phenomenon^{7,8,29-31}. Here, the results of the linearized stability analysis are directly used in determining the important parameters in the atomization process. For easier use of the linear stability analysis results, the maximum growth rate, Ω , and corresponding wavelength, Λ , of the Kelvin-Helmholtz instability mode are expressed by curve-fits in terms of non-dimensional numbers as,

$$\Omega_{KH} \left[\frac{\rho_l a^3}{\sigma} \right]^{0.5} = \frac{(0.34 + 0.38 We_g^2)}{(1 + Oh)(1 + 1.4 Ta^{0.6})} \quad (3)$$

$$\frac{\Lambda_{KH}}{a} = 9.02 \frac{(1 + 0.45 Oh^{0.5})(1 + 0.4 Ta^{0.7})}{(1 + 0.87 We_g^{1.67})^{0.6}} \quad (4)$$

where We_g is the Weber number for the gas phase, $We_g = \frac{\rho |U - V|^2 d}{\sigma}$, Oh is the Ohnesorge number, $Oh = v_1 \sqrt{\frac{\rho_l}{\sigma a}}$ and Ta is the Taylor parameter, $Ta = Oh \sqrt{We_g}$. The liquid breakup is modeled by adding new child parcels and their size is determined by

$$r_c = B_0 \Lambda_{KH} \quad (5)$$

where B_0 is a model constant and set equal to 0.61. Simultaneously, the parent drop size is reduced by

$$\frac{da}{dt} = -\frac{(a - r)}{\tau} \quad (6)$$

where τ is a time constant and determined from

$$\tau = 3.726 B_1 a / \Lambda_{KH} \Omega_{KH} \quad (7)$$

Here the drop size constant $B_0 = 0.61$ and breakup time constant $B_1 = 10.0$ as recommended in Ref 7. Child parcels are released when the stripped mass removed from the parent parcel exceeds a few percent of the average injected parcel mass.

Lastly, for high Weber number ($We > 350$) the Rayleigh-Taylor (RT) model³⁰ is applied with KH model. RT model is based on drop acceleration normal to the interface between two fluids that can drive the instability. Taking the external force acting on the droplet to be given by the aerodynamic drag, the acceleration can be expressed by dividing the drag force by the droplet mass:

$$a = \frac{3}{8} C_D \frac{\rho_g u_r^2}{\rho_l r} \quad (8)$$

Based on the linearized instability analysis by Chang³², the wavelength and frequency of the fastest growing waves are determined as:

$$\Lambda_{RT} = 2\pi \sqrt{\frac{3\sigma}{a\rho_l}} \quad (9)$$

$$\Omega_{RT} = \sqrt{\frac{2a}{3}} \left[\frac{a\rho_l}{3\sigma} \right]^{1/4} \quad (10)$$

The droplet breakup is allowed to occur when the RT wavelength, Λ_{RT} , is smaller than the droplet diameter until the RT breakup time, $\tau_{RT} = 1/\Omega_{RT}$.

C. Computational Geometry and Operating Conditions

The geometry of the single LDI element used in the simulation is shown in Fig. 2, which is the same as the one that was used in the companion experiments. The choked inlet slots (Detail A) and an exit nozzle (Detail C) are used to guarantee acoustically reflecting boundary conditions to sustain combustion instabilities in both the simulations and the experiments. Fuel injector (Detail B) sits in the converging-diverging section connecting the air plenum and combustor with the swirler. Preheated air comes through the choked inlet slots and enters the converging-diverging section through the air plenum. Hot air mixes with fuel spray from the fuel injector near the swirler and reacts in the combustor. The length of the air plenum and combustor are adjusted so that it supports a 3/8 acoustic wave in the air plenum and 1/2 wave in the combustor. This configuration has been reported to show lowest pressure oscillations in the experimental parametric studies by Gejji et al.³. Operating conditions for the simulations in this paper are focused at the high inlet air temperature ($T_{air} = 800K$) and high equivalence ratio ($\Phi = 0.6$) case with the fuel nozzle located at the venturi throat. As shown in Fig. 1, this condition has proven to be challenging for obtaining reliable computational predictions of the observed combustion instabilities and therefore serves as a good test case for the spray model evaluation and calibration studies.

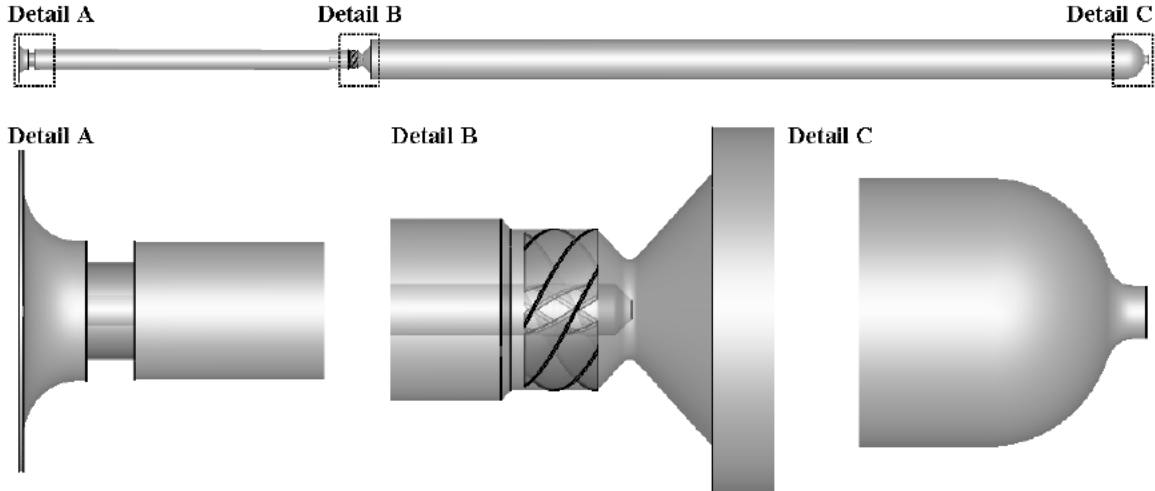


Figure 2. Computational geometry of LDI gas turbine combustor.

III. Results

In this section, investigations of fuel spray modeling effects are performed at the two physical stages of fuel spray corresponding to the primary and secondary atomization processes described in part B of section II. The predicted pressure signal is compared with the measured one to access the modeling effects. Further, for each study, the influence of model is further investigated by comparing the spray characteristics, gaseous fuel and heat release distributions.

As shown in Fig.1, the simulations with the fuel nozzle upstream of the throat provides better agreement with the experimental measurements and, therefore, it is useful to compare this case with the one where the fuel nozzle is at throat to help understand the possible modeling issues. The comparisons are focused on the heat release distribution, axial velocity and spray characteristics as shown in Fig. 3. The background contours are heat release rate (left) and axial velocity (right). The radius of drop is represented by the spray drop size in the figure and the colors on the spray drops represent the magnitude of temperature (left) and Weber number (right). One black iso-line of stoichiometric gaseous fuel mass fraction is used to indicate the distribution of vaporized gaseous fuel.

In Fig. 3, it can be observed that there are more spray drops left in the venturi when fuel nozzle is located at throat. Lots of small-size drops are observed in between the middle of diverging section and the dump plane, indicating a slow breakup process and vaporization, which can be attributed, in turn, to the insufficient spray drop breakup described by the models. Therefore, TAB and KH secondary breakup models are studied individually first by tuning the model constants to reduce the drop size after secondary breakup and also to accelerate the breakup process. Results from secondary breakup model constants tuning are shown in part A.

It is also noted in Fig. 3 that the Weber number of drops are higher with fuel nozzle upstream than at the throat and the fuel spray models described in part B of section II (primary: LISA and secondary: TAB/KH/RT) are highly Weber number dependent. Because of the sensitivity of spray modeling to Weber number, a small discrepancy may cause a large deviation in the spray predictions, which consequently affects the gaseous fuel production and heat release distributions. Hence, instead of applying a primary model, we look to specify a spray drop distribution which can be tuned to obtain reasonable combustion instability predictions. The effects of specified spray drop distribution are discussed in part B.

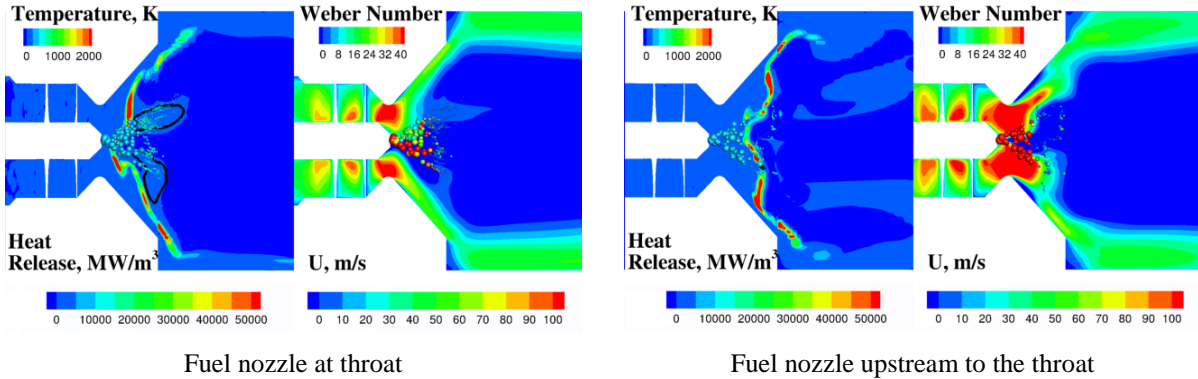


Figure 3. Instantaneous heat release distribution, axial velocity and spray characteristics comparisons between simulations with fuel nozzle at throat and upstream to the throat.

A. Effects of Secondary Breakup Model

Both TAB and KH/RT models are applied and tuned individually to systematically assess the effects of secondary breakup model. The discussion is mainly focused on the tuning of KH/RT model.

a. Tuning of TAB model

Due to the fact that TAB model has five independent controlling model constants, tuning of TAB model can largely make the evaluation difficult and so here only one constant C_f is selected for simplicity. In Eq. (2), by increasing the value of C_f , the value of We_C is increased, which increases the possibility of TAB-type of breakup process to occur. The tuning effects of TAB model on the pressure signal predictions are summarized in Table 2 and the computed pressure signals by tuning C_f value are shown and compared in Fig. 4. Comparing the Case A1 here and Case 4 in Table 1 (which model corresponds to the pressure signal results shown in bottom of Fig. 1), small improvements in predicted pressure amplitude can be observed and the 3L acoustic mode is more dominant in PSD plot. Increasing C_f to 1.0 helps improve the pressure prediction but further improvement cannot be achieved when C_f is further increased to 2.0, in which case the 1L mode starts to dominate over the 3L response. Overall, tuning the value of C_f is shown to have small improvements on the predictions but the overall effects are insignificant as evident in the pressure time histories and PSD's shown in Fig. 4.

Operating Conditions	Case Name	Total peak-to-peak pressure amplitude (%)	Dominant Acoustic Mode	Secondary Atomization Model
$T_{air} = 800K,$ $\Phi = 0.6$	Case A1: Baseline $C_f = 1/3$	0.7	3L	TAB
	Case A2: $C_f = 1.0$	0.8	3L	
	Case A3: $C_f = 2.0$	1.0	1L	

Table 2. Summary of TAB model tuning effects on pressure signal predictions.

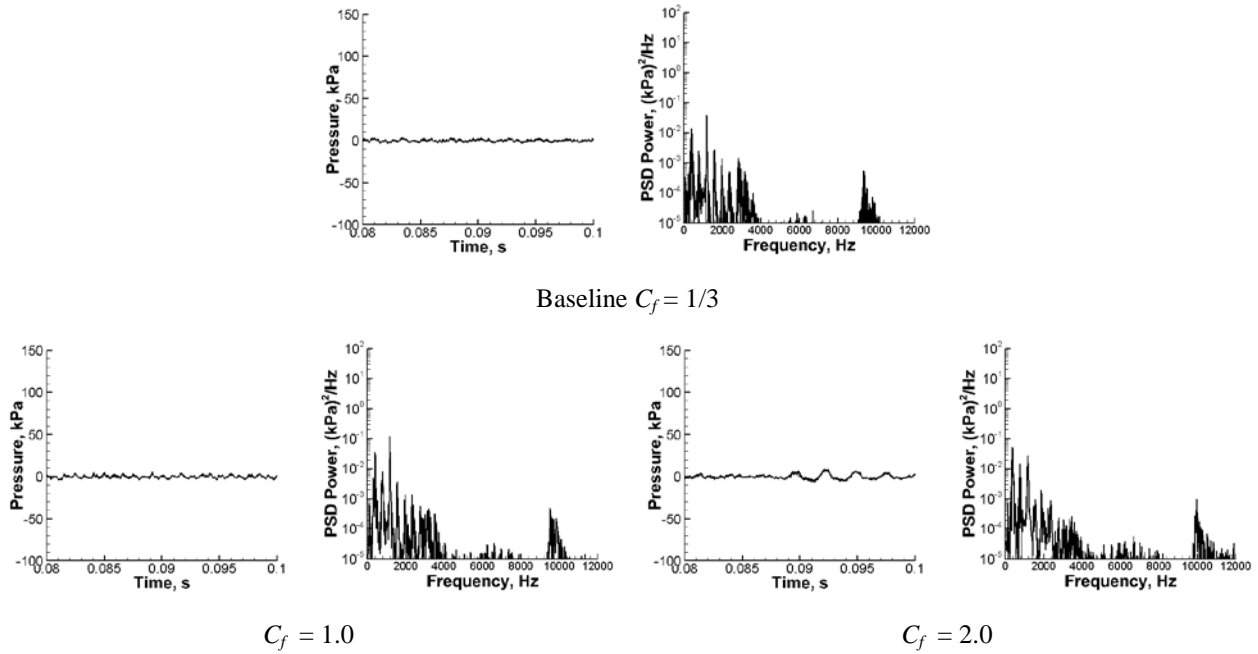


Figure 4. Comparisons of TAB model constants tuning effects on pressure predictions.

b. Tuning of KH model

The two model constants B_0 and B_1 in the KH model are varied to promote more secondary breakup. The constant B_0 controls the child drop size after breakup as shown in Eq. (5) and B_1 determines the breakup time in Eq. (7). By decreasing B_0 , the size of the child drops after secondary breakup is expected to decrease; while, by decreasing the value of B_1 , the secondary breakup process is expected to be faster. Both of these effects are aimed at

accelerating the secondary breakup process, thereby decreasing the child drop size and generating more gaseous fuel in the chamber for combustion.

Operating Conditions	Case Name	Total peak-to-peak pressure amplitude (%)	Dominant Acoustic Mode	Secondary Atomization Model
$T_{\text{air}} = 800\text{K}$, $\Phi = 0.6$	Case B1: Baseline $B_0 = 0.61$, $B_1 = 10.0$	0.5	3L	KH/RT
	Case B2: $B_0 = 0.5$, $B_1 = 10.0$	0.7	3L	
	Case B3: $B_0 = 0.2$, $B_1 = 10.0$	1.1	1L	
	Case B4: $B_0 = 0.61$, $B_1 = 2.0$	0.7	3L	

Table 3. Summary of KH model tuning effects on pressure signal predictions.

The KH model tuning effects are summarized in Table 3 and the predicted pressure comparisons are shown in Fig. 5. By using only the KH/RT model to describe secondary atomization, the baseline case (Case B1) shows a small improvement in capturing the dominant 3L frequency compared with the hybrid model (Case 4) in Table 1. As discussed in part a, using only the TAB model also improved the prediction slightly. These results may therefore indicate some inherent limitations of hybrid model in combining TAB and KH/RT models based on the Weber number.

The first tuning step is to decrease the value of B_0 while keeping B_1 the same (Case B2 and Case B3); this leads to a nominal pressure amplitude increase and, eventually, the 1L acoustic mode becomes more excited than the 3L mode. The second step is to decrease the value of B_1 to accelerate the spray breakup (Case B4). Again, the predicted pressure amplitude increases somewhat with the 1L and 3L appearing as the most two dominant modes observed in the PSD plot in Fig. 5. However, the overall effects in improving combustion instability predictions are not significant and the simulations still underpredict the pressure amplitude compared with experimental measurements.

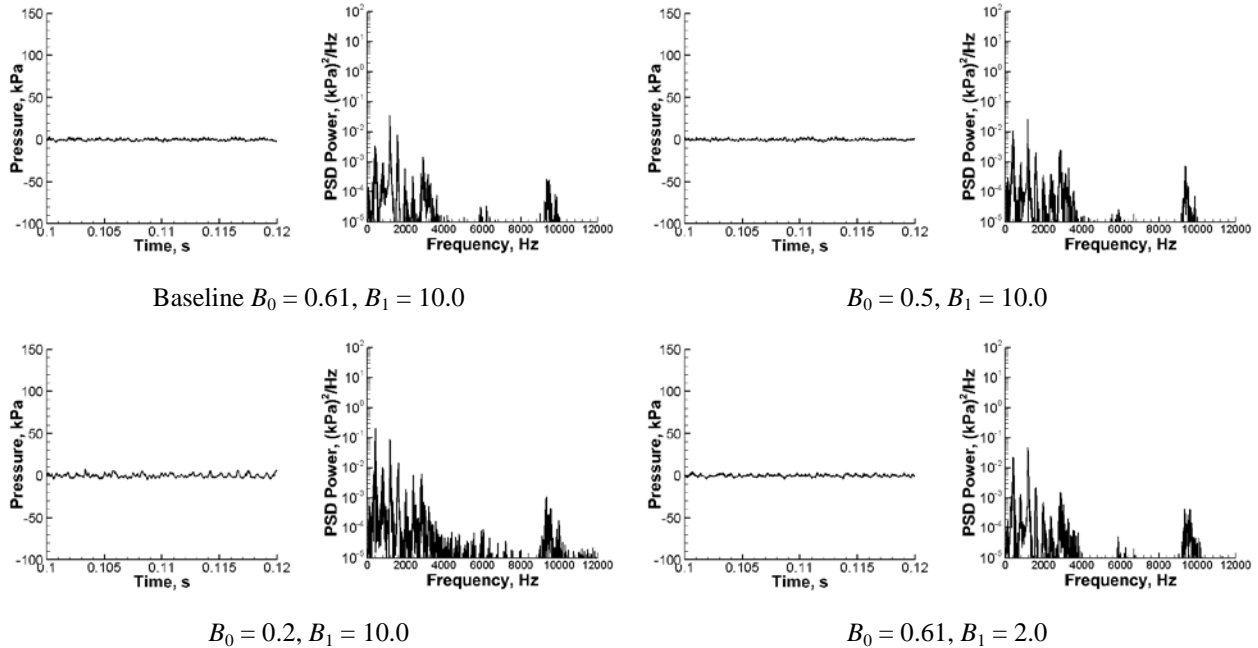


Figure 5. Comparisons of KH model constants tuning effects on pressure predictions.

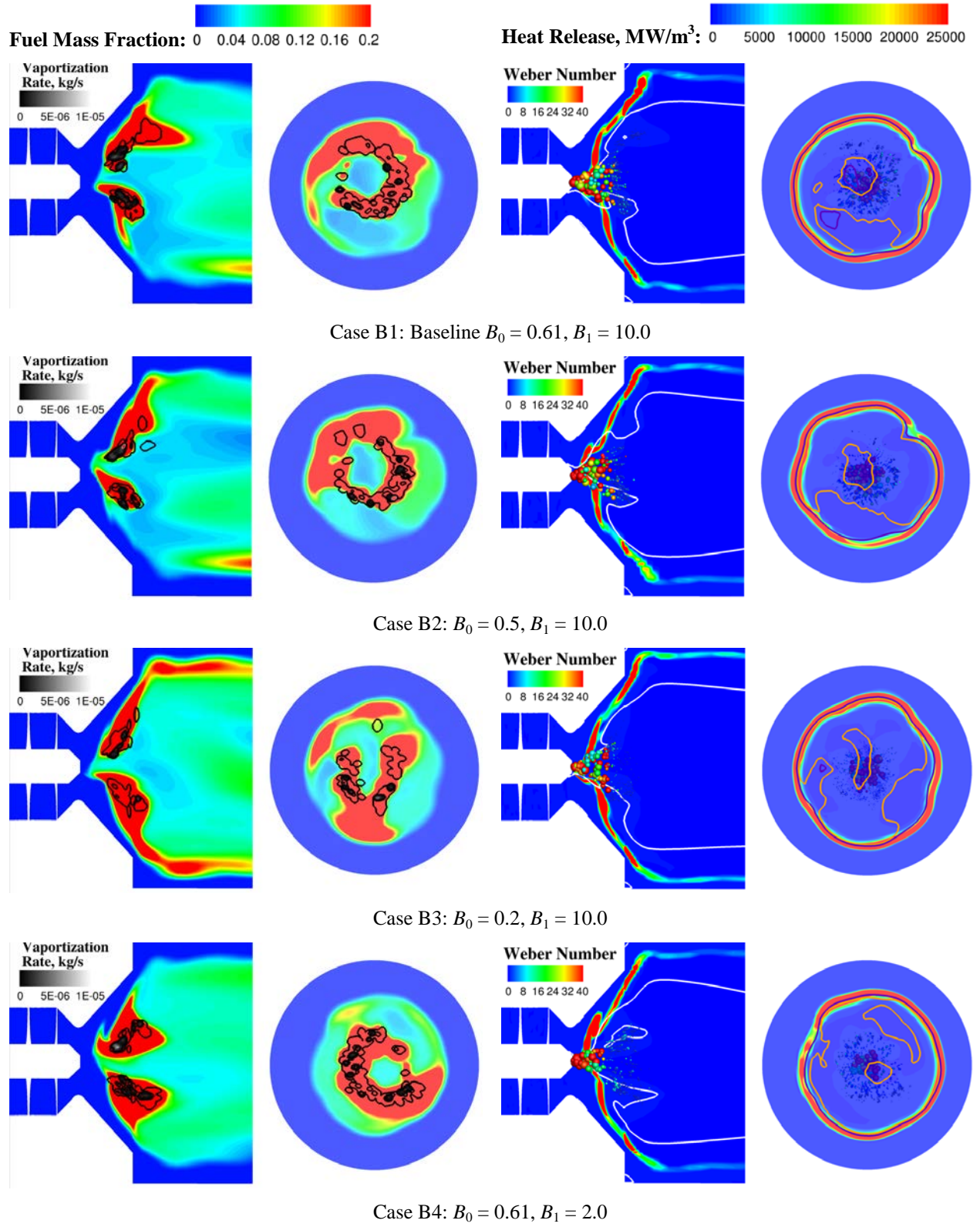


Figure 6. Comparisons of KH model constants tuning effects on predictions of vaporized fuel and heat release distribution.

To further understand the effects of model tuning and to help guide fuel spray modeling improvements, the spray characteristics, gaseous fuel mass fraction and heat release rate distributions are compared for different KH model constants and are shown in Fig. 6. The vaporized fuel mass fraction is shown as the background rainbow contour and the vaporization rate is shown as contour lines in grey scale in the left column. The heat release is shown as the background rainbow contour with fuel spray drops colored by the Weber number. An iso-line of zero axial velocity is highlighted in white to represent the Vortex Breakup Bubble (VBB), which was determined to be responsible for the major mechanism to sustain combustion instability in the LDI combustor¹⁶. A cross-sectional view is selected 1mm downstream of the dump plane to visualize the three-dimensional effects in each figure and iso-lines of gaseous fuel mass fraction are overlapped in heat release contour.

In the side view, the spatial distributions of the vaporization rates for all four cases look similar and follow the hollow cone configuration as specified by the fuel spray injection with a cone angle around 65° . In the cross-sectional view, the spatial distributions of the vaporization rate show a spiral structure, which is driven by the strong swirling flow generated by the swirler upstream. Cases B1 and B2 have similar asymmetric gaseous fuel distributions in the side view and similar spiral structures as the vaporization rate in cross-sectional view.

In Case B3, the fuel distribution is more symmetric and stretched in the side view. Moreover, with reduced model constant B_0 , it can be seen that more small-size drops with lower Weber number are generated in the chamber compared with Case B1 and B2. Those small drops can be easily driven by the flow-field, following the VBB outline and vaporizing in downstream locations. This is probably the reason that the gaseous fuel distribution in Case B3 assembles the shape of the VBB and more fuel is present in the chamber.

In Case B4, the fuel distribution is also different from the other three cases. With model constant B_1 reduced, the secondary atomization process occurs faster and consequently even more small-size drops are generated than in Case B3. This accelerated KH breakup model produces small drops at a high rate, which in turn limit the time for the flow-field to interact with the small drops and therefore the gaseous fuel distribution here is more compact and more restricted to the diverging section.

Though differences can be observed in the fuel distributions and spray characteristics by tuning the KH model constants, the heat release distributions look very similar for all four cases and the tuning effects on the VBB are also not very significant, which explains why the improvements in pressure predictions (in Fig. 5) are not significant either. These results suggest that stronger effects may arise in the early stages of fuel spray formation such as the free surface flow inside fuel injector and the primary atomization process. Accordingly, the results in the next section are focused on the effects of primary atomization on the fuel spray distribution.

B. Effects of Fuel Spray Distribution

Instead of including a primary breakup model, a specified fuel spray distribution with hollow cone configuration is applied in order to systematically assess the effects of fuel spray distribution on combustion instability predictions. In these studies, the hybrid model is retained to describe secondary atomization. The types of distributions and their effects on the pressure predictions are summarized in Table 4 and the predicted pressure signals are shown in Fig. 7. Compared with the tuning studies of secondary breakup models, it is apparent that the improvements on pressure signal predictions by specifying a drop distribution are more significant.

Operating Conditions	Case Name	Total peak-to-peak pressure amplitude (%)	Dominant Acoustic Mode	Secondary Atomization Model
$T_{\text{air}} = 800\text{K}$, $\Phi = 0.6$	Case C1: Uniform spray distribution ($d_{\text{mean}} = 78 \mu\text{m}$)	20	3L/1T	Hybrid TAB/KH/RT
	Case C2: Log-normal spray distribution ($d_{\text{mean}} = 56 \mu\text{m}$)	4	4L	
	Case C3: Log-normal spray distribution ($d_{\text{mean}} = 78 \mu\text{m}$)	1.5	3L	
	Case C4: Log-normal spray distribution ($d_{\text{mean}} = 156 \mu\text{m}$)	8	1T1L	

Table 4. Summary of fuel spray distribution effects on pressure signal predictions

The predicted pressure signal seems to be very sensitive to the specified fuel spray distribution based on Table 4 and Fig. 7. By using a uniform fuel spray distribution with mean diameter as $78\text{ }\mu\text{m}$ (Case C1), which is comparable to the liquid sheet thickness obtained from the offline VOF computation described in part B of section II, the predicted pressure amplitude is getting closer to experiment measurement (summarized in Table 1). The 3L is dominant which is close to the 4L mode observed in the experiments. However, the response at 1T has been over-predicted while the frequencies that lie in between the 3L and 1T modes are under-predicted.

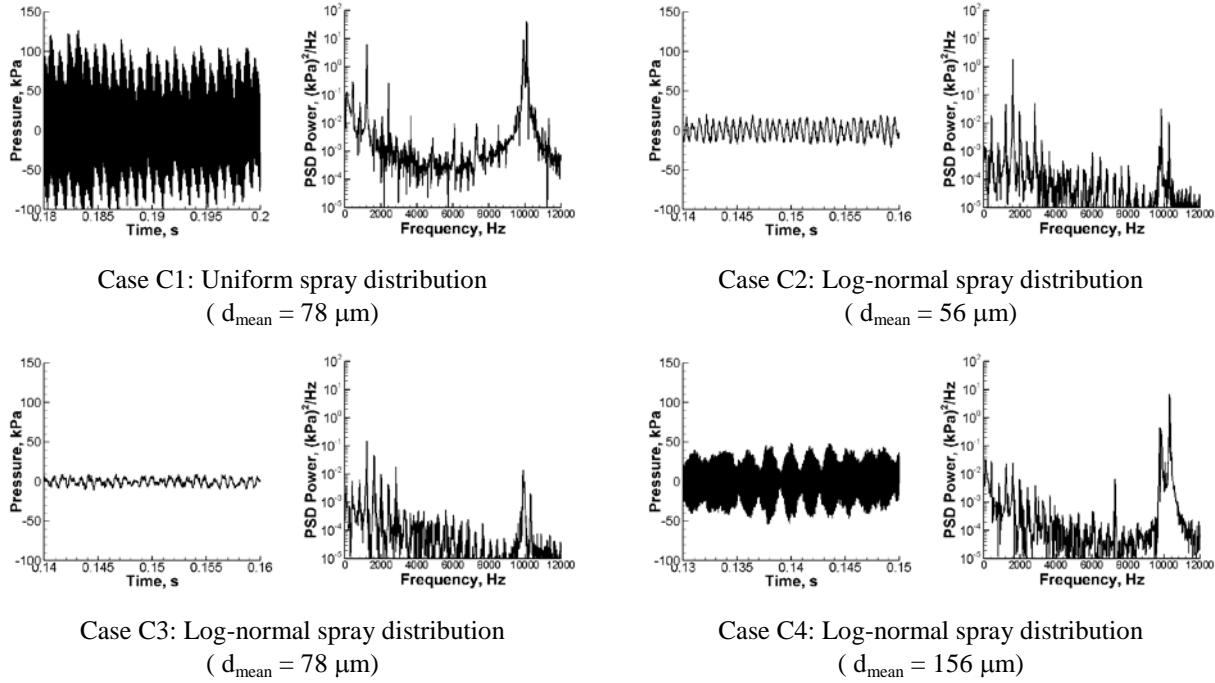


Figure 7. Comparisons of fuel spray distribution on pressure predictions

By using a log-normal distribution with a mean diameter of $56\text{ }\mu\text{m}$ (which is comparable to drop size measured from atmospheric spray experiment¹²), the dominant acoustic frequency shifts to the 4L mode in agreement with the experiments, but the pressure amplitude is under-predicted (Case C2). Moreover, increasing the mean diameter in the log-normal distribution does not help improve the pressure predictions. Case C3 predicts the 3L mode as the dominant frequency but the pressure amplitude is even lower than Case C2. Further doubling the mean drop size (Case C4), the prediction in pressure amplitude is improved and getting closer to the experimental measurements, but 1T-1L acoustic mode is observed to be the most dominant mode while the contributions of the longitudinal acoustic modes are significantly under-predicted.

Detailed comparisons on the fuel spray distribution effects are shown in Fig. 8. The contents of these plots are similar to the plots in Fig. 6. The distributions of gaseous fuel mass fraction, heat release and spray characteristics are studied specifically. One major difference due to the replacement of the primary breakup LISA model with a specified drop distribution is that the heat release level has been increased significantly, which is probably related to why the predicted pressure oscillation amplitudes have been improved. With more unsteady heat release coupled with pressure fluctuations, the driving of instability becomes stronger. Moreover, another important difference is that the spray drop sizes left in the domain in Cases C1 and C3 are much smaller than those in Cases B1 - B4. It should be noted that the initial drops injected to the chamber are of similar size ($\sim 78\text{ }\mu\text{m}$) for these cases. This indicates that the LISA model under-predicts the spray breakup process. More importantly, it indicates the great degree of sensitivity of combustion instability predictions to local spray drop distribution, breakup and vaporization phenomena.

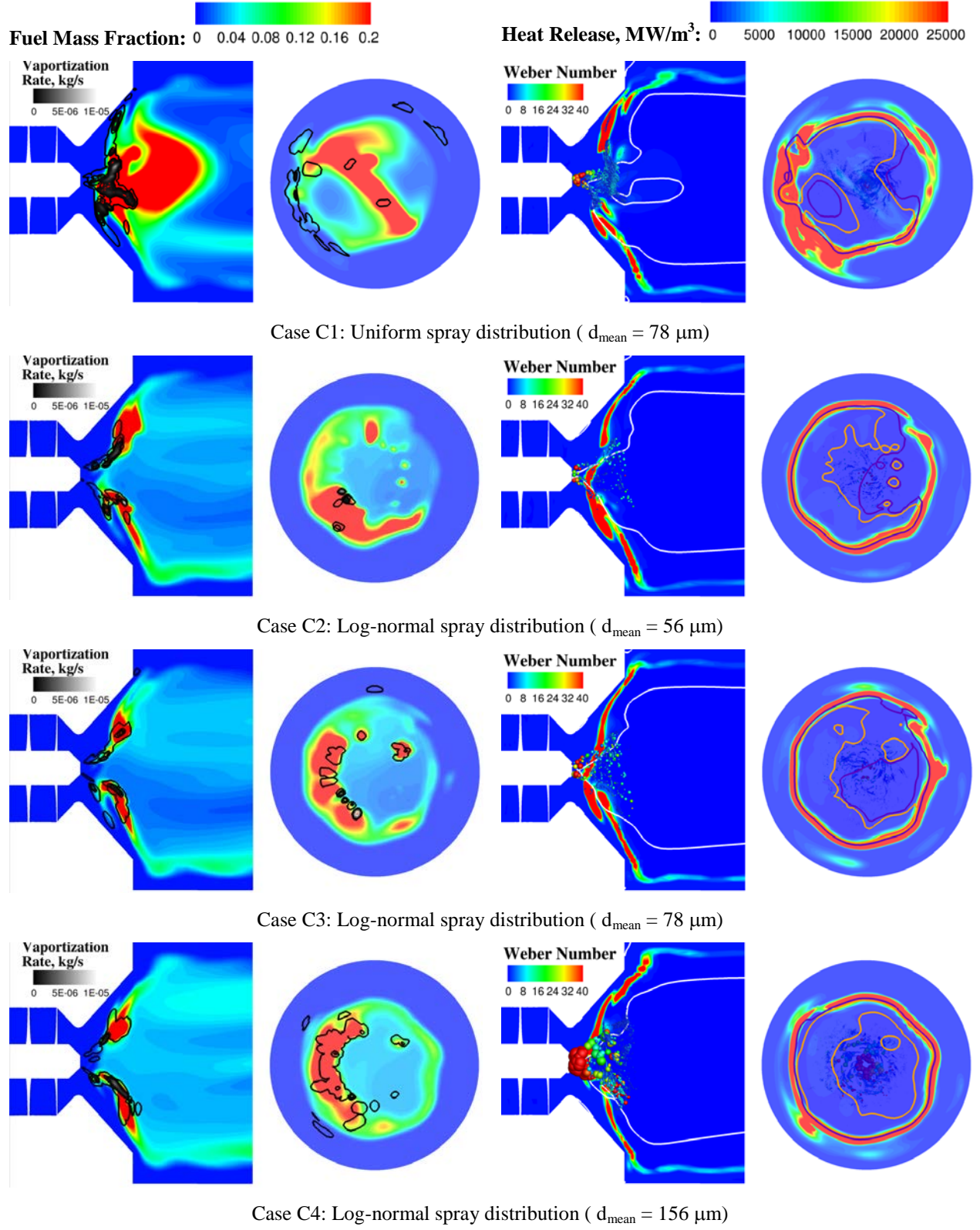


Figure 8. Comparisons of fuel spray distribution on predictions of vaporized fuel and heat release distributions.

Very different behavior can also be observed by comparing results using uniform drop distribution and those using a log-normal distribution. For the uniform distribution case (C1), the high vaporization rate is concentrated near the central region, which generates large amount of gaseous fuel there while, for all the log-normal distribution cases (C2, C3 and C4), the vaporization rates follow a hollow-cone-like structure (consistent with the spray injection configuration). Also, the heat release rate in Case C1 is much lower in the center region where fuel is rich and it is more concentrated in space while the log-normal distribution cases predict a more extended and stretched flame. The concentrated heat release distribution can be the reason why the predicted pressure amplitude is higher when using uniform distribution. In addition, an intact VBB can be observed in Case C1, which weakens the center reversing flow and allows the vaporized fuel to accumulate. In contrast, for the other cases, the VBB structure is complete and strong reversing flow in the center forces the vaporized fuel to follow the bubble outline and form a conical shape. It is therefore evident that the type of spray drop distribution can be critical for determining the predicted flow-field and the associated combustion response.

Cases C2 - C4 use the log-normal distribution but the mean drop diameter is varied. Other than the difference in the spray drop size, these three cases predict similar spatial distributions of the vaporized fuel mass fraction, spray vaporization rate and heat release but interestingly show very different instability behaviors as summarized in Table 4 and Fig. 7. This indicates the strong sensitivity of predicted pressure oscillations to the mean spray drop size. As shown in Fig.1 (bottom left), a very rich frequency spectrum has been found in the measured pressure signal. Therefore, small changes in the spray distribution can trigger a different mode of coupling of the unsteady combustion response with any specific frequency in the spectrum.

Overall, replacing the primary breakup model with a specified spray drop distribution and applying some moderate amount of adjustment in distribution are seen to have significant effects in combustion instability predictions. However, the predictions can be very sensitive to the distribution specified and the distribution adjustment needs to be performed very carefully to reach reasonable agreement with the experimental measurement. More specifically, these results point to the need for more directly coupled ab initio models of the atomizer free surface flow and the primary atomization processes, thereby avoiding ad hoc assumptions of droplet distributions that are likely to be problem-dependent.

IV. Conclusions and Future Work

The effects of fuel spray modeling on predictions of self-excited combustion instability are evaluated using computational results in a single-element laboratory LDI gas turbine combustor. Previous studies used the LISA primary breakup model plus the Weber number based hybrid secondary atomization model (comprised of the TAB/KH/RT models). The simulations showed good agreement with experimental measurements when the fuel nozzle is located upstream of the venturi throat, while the pressure amplitude was under-predicted when the fuel nozzle is at the venturi throat. Based on comparisons between the two cases, it is postulated that the insufficiency in spray drop breakup and under-predicted Weber number can be the major causes for the prediction discrepancies. To improve the simulation predictions, two steps of modeling assessment are performed in terms of secondary breakup and primary breakup physical processes.

Model constants tuning has been conducted for both TAB and KH models. The constants are tuned to either reduce the drop size after breakup or to accelerate the breakup time. For both models, the tuning indicates small improvements in the predictions, but the overall effects are not significant enough. This indicates that tuning of secondary breakup model has less significant effects on combustion instability predictions, suggesting that the dominant effects may lie earlier in the spray formation process.

As a second step in the study, the LISA model was replaced by a specified fuel spray distribution to assess the effects of fuel spray distributions on combustion instability predictions. Two types of distributions were applied---a uniform spray distribution and a log-normal distribution. In both cases, the amplitudes of the predictions are improved significantly, but no specific distribution is capable of simultaneously predicting the correct overall amplitudes as well as the correct dominant instability modes.

Detailed investigations of the computed spray characteristics, vaporized fuel and heat release distributions for the different cases show significant differences in the droplet sizes and vaporized fuel concentrations, which explain many of the observed trends. This high degree of sensitivity of the predicted distributions and the associated combustion response to the spray model suggests the importance of using more ab initio models for capturing the

spray formation phenomena. In this regard, the coupled Level Set/VOF approach presents a promising direction for future study³³.

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